A New Method for Predicting the Liquid Heat Capacity of Pure Components

J.L. Oscarson, C.C. Stingel, R.L. Rowley, and W.V. Wilding
Department of Chemical Engineering
Brigham Young University
Provo, UT U.S.A.

Liquid heat capacities are needed in order calculate the energy requirements of industrial processes. In general, the methods used to predict heat capacities of liquids are not very accurate. On the other hand, methods have been developed that can predict heat capacities of ideal gases with good accuracy. The best of these methods are group-contribution methods. The basis for these methods is the assumption that the contribution of a specific group to the heat capacity is the same in all compounds in which it is a constituent. In liquids there is a strong inter-molecular interaction. This interaction is difficult to predict using group-contribution methods. A method that uses predicted ideal-gas heat capacities, measured vapor pressures, and an equation of state to predict liquid heat capacities has been investigated. This method uses the Clapeyron equation to predict the heat of vaporization of the fluid using vapor pressures. Once the heat of vaporization as a function of temperature is established, the heat capacity of the liquid at saturation C_σ (liq) is found using the heat capacity of the vapor at saturation C_σ (vap) and the temperature derivative of the heat of vaporization. Equations of state are used to convert these heat capacities to heat capacities of the liquid and ideal gas at constant pressure. It has been found that the answer is highly dependent on the correlating equations used to fit the vapor pressures and heat of vaporization. The correlating equations that work best and the method will be explained and the results for several classes of compounds will be shown.